

# Creating custom protocols with ROSETTA

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ROSETTA Workshop

4/26/2017

# Custom Protocols

- Rosetta applications cover most common tasks
- Sometimes you want to do something different
  - Modify an existing protocol
  - Combine two protocols
  - Make an entire novel protocol

# How to Make Custom Protocols

- C++ - Directly modify the Rosetta source code
- PyRosetta – Python bindings for directly interacting with Rosetta functions (<http://www.pyrosetta.org/>)
- RosettaScripts – XML based interface for creating protocols

# Structure of ROSETTA XML file

```
<ROSETTASCRIPTS>  
  <SCOREFXNS>  
  </SCOREFXNS>  
  <FILTERS>  
  </FILTERS>  
  <TASKOPERATIONS>  
  </TASKOPERATIONS>  
  <MOVERS>  
  </MOVERS>  
  <PROTOCOLS>  
  </PROTOCOLS>  
  <OUTPUT />  
</ROSETTASCRIPTS>
```

- XML “eXtensible Markup Language”
- Widely used for representing hierarchical data
- Rosetta supports a variant of XML – recently overhauled to fulfill XML standards

# Movers

```
<MOVERS>
```

```
<PackRotamersMover name="repack1" scorefxn="score12_002" taskoperations="ifcl,rtrp" />
```

```
<PackRotamersMover name="repack2" scorefxn="score12_005" taskoperations="ifcl,rtrp" />
```

```
<PackRotamersMover name="repack3" scorefxn="score12_055" taskoperations="ifcl,rtrp" />
```

```
<InterfaceAnalyzerMover name="iface" scorefxn="score12" fixedchains="A,B" />
```

```
</MOVERS>
```

- Movers are the basic building blocks of a RosettaScripts protocol
- Most modify the pose
  - Some compute metrics instead
- A single mover can be used more than once

# Filters

```
<FILTERS>
```

```
  <ScoreType name="score_type_filter" scorefxn="score12" score_type="total_score"  
Threshold="-500" />
```

```
  <AverageDegree name="avg_deg" threshold="8" distance_threshold="10"  
task_operations="rtiv" />
```

```
</FILTERS>
```

- Can pass/fail an output structure
  - Stop a run earlier if the output will be bad.
- Also can be used to compute protein metrics

# Score Functions

```
<SCOREFXNS>  
  <ScoreFunction name="ligand_soft_rep" weights="ligand_soft_rep" />  
  <ScoreFunction name="hard_rep" weights="ligand">  
    <Reweight scoretype="fa_intra_rep" weight="0.004"/>  
    <Reweight scoretype="fa_elec" weight="0.42"/>  
  </ScoreFunction>  
</SCOREFXNS>
```

- Different parts of a protocol can use different score functions
- Standard score functions can be modified

# Task Operations

```
<TASKOPERATIONS>
```

```
  <ReadResfile name="rrf" filename="resfile" />
```

```
  <RestrictToRepacking name="rtrp" />
```

```
  <RestrictResidueToRepacking name="restrict_Y100" resnum="100" />
```

```
</TASKOPERATIONS>
```

- Select residues
- Specify how to allow sidechain movement
- Specify which residues to allow to design



# Protocols

```
<PROTOCOLS>  
  <Add mover="Repack1"/>  
  <Add mover="Repack2" filter="avg_deg" />  
  <Add mover="iface"/>  
</PROTOCOLS>
```

- Movers are executed in the order specified in PROTOCOLS
- Movers can be combined with filters
- Movers can be used more than once in a protocol

# Output

```
<OUTPUT scorefxn="talaris2014" />
```

- Specifies the score function used for the final output model and in the scorefile
- If you use multiple score functions in a protocol or use a non-default score function – make sure to flag this!

# Executing Protocols

```
rosetta_scripts.default.linuxgccrelease @options.txt -parser:protocol  
protocol.xml
```

- RosettaScripts protocols are run using the rosetta\_scripts application
- All the normal file IO options are supported
- Some movers have their own associated command line options

# Documentation

## RosettaScripts

[https://www.rosettacommons.org/docs/latest/scripting\\_documentation/RosettaScripts/RosettaScripts](https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/RosettaScripts)

## Movers

[https://www.rosettacommons.org/docs/latest/scripting\\_documentation/RosettaScripts/Movers/Movers-RosettaScripts](https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Movers/Movers-RosettaScripts)

## Filters

[https://www.rosettacommons.org/docs/latest/scripting\\_documentation/RosettaScripts/Filters/Filters-RosettaScripts](https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/Filters/Filters-RosettaScripts)

## Task Operations

[https://www.rosettacommons.org/docs/latest/scripting\\_documentation/RosettaScripts/TaskOperations/TaskOperations-RosettaScripts](https://www.rosettacommons.org/docs/latest/scripting_documentation/RosettaScripts/TaskOperations/TaskOperations-RosettaScripts)